

## CAS ONLINE PRINTOUT

=&gt; d his

(FILE 'HOME' ENTERED AT 12:00:24 ON 02 MAR 2006)

FILE 'REGISTRY' ENTERED AT 12:01:08 ON 02 MAR 2006

L1 STRUCTURE UPLOADED  
L2 50 S L1  
L3 1321 S L1 FUL  
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L5 STRUCTURE UPLOADED  
L6 0 SEARCH L5 SSS SUB=L3 FUL  
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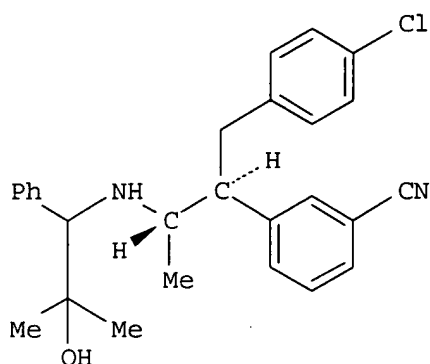
FILE 'CAPLUS' ENTERED AT 12:09:30 ON 02 MAR 2006

L13 33 S L12

=&gt; d bib abs hitstr 1-33

L13 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2005:429387 CAPLUS  
DN 142:481820  
TI Preparation of aralkyl amines as cannabinoid-1 receptor modulators  
IN Shah, Shrenik K.; Truong, Quang T.; Qi, Hongbo; Hagmann, William K.  
PA Merck & Co., Inc., USA  
SO PCT Int. Appl., 137 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005044785	A1	20050519	WO 2004-US35846	20041027
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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PRAI	US 2003-515705P	P	20031030		
OS	MARPAT 142:481820				
GI					

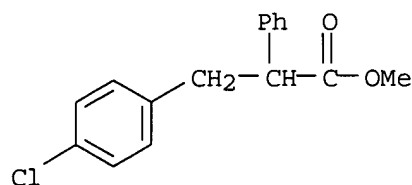


AB Aralkyl amines ((Ar1X)C(R1)(Ar2)CH(R2)N(R3)C(R4)(R5)Ar3 (I); variables defined below; e.g. 2 diastereomers of 3-[1-(S\*)-(4-chlorobenzyl)-2-(S\*)-[[2-hydroxy-2-methyl-1-(R\*)-phenylpropyl]amino]propyl]benzonitrile (shown as II)) are antagonists and/or inverse agonists of the Cannabinoid-1 (CB1) receptor and are useful in the treatment, prevention and suppression of diseases mediated by the CB1 receptor. The compds. of the present invention are useful as centrally acting drugs in the treatment of psychosis, memory deficits, cognitive disorders, migraine, neuropathy, neuro-inflammatory disorders including multiple sclerosis and Guillain-Barre syndrome and the inflammatory sequelae of viral encephalitis, cerebral vascular accidents, and head trauma, anxiety disorders, stress, epilepsy, Parkinson's disease, movement disorders, and schizophrenia. The compds. are also useful for the treatment of substance abuse disorders, including alc. and nicotine addiction, the treatment of obesity or eating disorders, as well as the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver. For I: R1 = H, Cl-4alkyl, (un)substituted with 1-3 Re, halogen, and -ORD; R2 = H, Cl-4alkyl, and aryl, wherein each alkyl and aryl moiety is (un)substituted with 1-3 Re; R3 = H, and Cl-4alkyl, (un)substituted with 1-3 Re; R4 = H, Cl-10alkyl, C2-10alkenyl, C2-10alkynyl, Cl-10alkyloxycarbonyl-, C3-10cycloalkyl, aryl-Cl-6alkyl-, and heteroaryl-Cl-6-alkyl-, wherein each alkyl, alkenyl, and alkynyl moiety is (un)substituted with 1-4 Ra and each aryl, heteroaryl, and cycloalkyl moiety is (un)substituted with 1-3 Rb and oxo; R5 = H, and Cl-4alkyl, (un)substituted with 1-3 Re. Ar1 = Cl-10alkyl, C2-10alkenyl, C2-10alkynyl, C3-10cycloalkyl, cycloheteroalkyl, aryl, and heteroaryl, wherein each alkyl, alkenyl, and alkynyl moiety is (un)substituted with 1-3 Ra, each aryl and heteroaryl moiety is (un)substituted with 1-4 Rb and each cycloalkyl and cycloheteroalkyl moiety is (un)substituted with 1-4 Rb and oxo; Ar2 = -ORD, -CO2Rd, C3-10cycloalkyl, cycloheteroalkyl, aryl, and heteroaryl, wherein each cycloalkyl, cycloheteroalkyl moiety is (un)substituted with 1-4 Rb and oxo and each aryl and heteroaryl moiety is (un)substituted with 1-4 Rb; Ar3 = cycloalkyl, aryl, and heteroaryl, wherein each cycloalkyl, aryl and heteroaryl moiety is (un)substituted with 1-4 Rb; X = a bond, Cl-4alkyl, O, S, and -NRC-, provided that when X is O, S, or -NRC-, then R1 is H or Cl-4alkyl and Ar2 is not -ORD; addnl. details are given in the claims. Although the methods of preparation are not claimed, >100 example preps. and/or characterization data for I are included. For example, II was prepared from [3-(4-chlorophenyl)-2-(S\*)-(3-cyanophenyl)-1-(S\*)-methylpropyl]amine, 2-hydroxy-2-methylpropiophenone and NaHB(OAc)3 in dichloroethane. Compds. I were tested in a CB1 binding assay and found to have an IC50 value of  $\leq 2 \mu\text{M}$ . Selective CB1 antagonist/inverse agonist compds. have IC50s 100-fold greater in the CB2 binding assay than in the CB1 assay, and generally have IC50s  $>1 \mu\text{M}$  in the CB2 binding assay. CB1 antagonist/inverse agonist compds. I generally

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have EC50s of <1  $\mu$ M in a CB1 functional assay and selective CB1 antagonist/inverse agonists generally have EC50s >1  $\mu$ M in the CB2 functional assay.

IT **92907-23-8P**, 3-(4-Chlorophenyl)-2-phenylpropanoic acid methyl ester  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of aralkyl amines as cannabinoid-1 receptor modulators)  
 RN 92907-23-8 CAPLUS  
 CN Benzenepropanoic acid, 4-chloro- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2005:281753 CAPLUS  
 DN 142:355050  
 TI Preparation of aryl sulfonamides as cannabinoid CB1 receptor antagonists and/or inverse agonists.  
 IN Armstrong, Helen M.; Chang, Linda L.; Guthikonda, Ravindra N.; Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.  
 PA Merck & Co., Inc., USA  
 SO PCT Int. Appl., 122 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005027837	A2	20050331	WO 2004-US30122	20040914
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	RW:				
	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI US 2003-504377P P 20030918

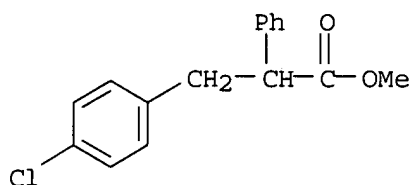
OS MARPAT 142:355050

AB R1R2R6CCR3R7NR4SO2R5 [I; R1 = (substituted) alkyl, cycloalkyl(alkyl), cycloheteroalkyl(alkyl), (hetero)aryl(alkyl), etc.; R2 = (substituted) alkyl, cycloalkyl(alkyl), cycloheteroalkyl(alkyl), (hetero)aryl(alkyl); R3, R7 = H, (substituted) alkyl, cycloalkyl(alkyl), (hetero)aryl(alkyl), cycloheteroalkyl(alkyl); R4 = H, (substituted) alkyl; R5 = (substituted) alkyl, alkenyl, alkynyl, cycloheteroalkyl(alkyl), cycloalkyl(alkyl), (hetero)aryl(alkyl), etc.; R6 = H, OH, alkyl, halo, cyano; with provisos], were prepared Thus, 2-amino-3,4-bis(4-chlorophenyl)butane hydrochloride,

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diisopropylethylamine, and tert-butylsulfinyl chloride were stirred together in CH<sub>2</sub>Cl<sub>2</sub> for 2 h to give N-[2,3-bis(4-chlorophenyl)-1-methylpropyl]-2-methyl-2-propanesulfinimide. This was stirred with m-ClC<sub>6</sub>H<sub>4</sub>C(O)OOH in CH<sub>2</sub>Cl<sub>2</sub> to give N-[2,3-bis(4-chlorophenyl)-1-methylpropyl]-2-methyl-2-propanesulfonimide. I generally have EC<sub>50</sub> values of <1 μM in a CB<sub>1</sub> functional assay.

IT **92907-23-8P**, 3-(4-Chlorophenyl)-2-phenylpropanoic acid methyl ester  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of aryl sulfonamides as cannabinoid CB<sub>1</sub> receptor antagonists and/or inverse agonists)  
 RN 92907-23-8 CAPLUS  
 CN Benzenepropanoic acid, 4-chloro-α-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 3 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2004:467848 CAPLUS  
 DN 141:38363  
 TI Preparation of propanamide derivatives as cannabinoid-1 receptor antagonists  
 IN Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.; Guthikonda, Ravindra N.; Qi, Hongbo; Chang, Linda L.; Liu, Ping; Armstrong, Helen M.; Jewell, James P.; Lanza, Thomas J., Jr.  
 PA Merck & Co., Inc., USA  
 SO PCT Int. Appl., 99 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004048317	A1	20040610	WO 2003-US7039	20030307
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	RW:				
	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	BR 2003008349	A	20050125	BR 2003-8349	20030307
	NO 2004003803	A	20050524	NO 2004-3803	20040910
PRAI	US 2002-428415P	P	20021122		
	WO 2003-US7039	W	20030307		
OS	MARPAT 141:38363				
AB	The title compds. with general formula of R <sub>1</sub> R <sub>2</sub> CH-CH(Me)-NH-CO-C(Me <sub>2</sub> )-O-R <sub>3</sub> [wherein R <sub>1</sub> = heterocyclyl, aryl, heteroaryl, (un)substituted amino, etc.; R <sub>2</sub> = alkyl, cycloalkylalkyl, arylalkyl, heteroarylalkyl, etc.; R <sub>3</sub> =				

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cycloalkyl, aryl, heteroaryl, etc.) or pharmaceutically acceptable salts thereof are prepared as cannabinoid-1 (CB1) receptor antagonists. For example, N-[2,3-bis(4-chlorophenyl)-1-methylpropyl]-2-(4-chlorophenoxy)-2-methylpropanamide was prepared in a multi-step synthesis. The compds. are useful for the treatment of substance abuse disorders, the treatment of obesity or eating disorders, as well as the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver (no data).

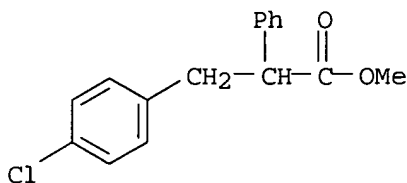
IT 92907-23-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of propanamide derivs. as cannabinoid-1 receptor antagonists)

RN 92907-23-8 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:837028 CAPLUS

DN 139:337785

TI Preparation of substituted arylamides as cannabinoid-1 receptor antagonists and/or inverse agonists for use as psychotropic drugs

IN Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.

PA Merck &amp; Co., Inc., USA

SO PCT Int. Appl., 191 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003087037	A1	20031023	WO 2003-US9800	20030401
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RW:				
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CA 2480856	AA	20031023	CA 2003-2480856	20030401
AU 2003226149	A1	20031027	AU 2003-226149	20030401
EP 1494997	A1	20050112	EP 2003-746565	20030401
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JP 2005527586	T2	20050915	JP 2003-583993	20030401

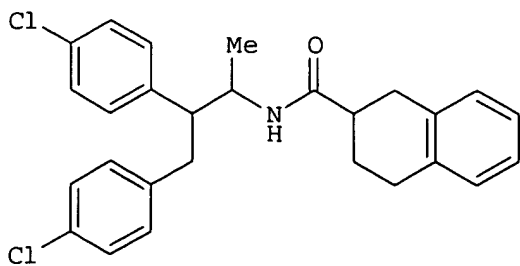
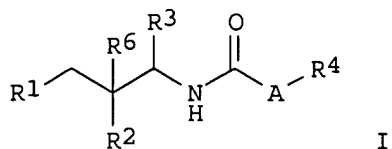


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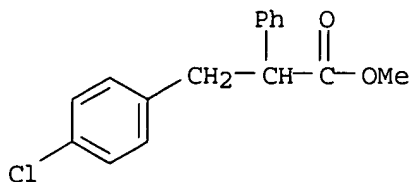
RE.CNT 3      THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2003:836767 CAPLUS  
DN 139:337784  
TI Preparation of substituted bicyclic arylamide cannabinoid-1 receptor  
antagonists and/or inverse agonists for use as psychotropic drugs  
IN Castonguay, Laurie A.; Hagmann, William K.; Lin, Linus S.; Shah, Shrenik  
K.  
PA Merck & Co., Inc., USA  
SO PCT Int. Appl., 189 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003086288	A2	20031023	WO 2003-US10740	20030408
	WO 2003086288	A3	20040805		
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EP	1499306	A2	20050126	EP 2003-719642	20030408
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US	2005203112	A1	20050915	US 2004-509584	20040929
PRAI	US 2002-372234P	P	20020412		
	WO 2003-US10740	W	20030408		
OS	MARPAT 139:337784				
GI					



- AB Title compds. I [wherein R1 = (un)substituted alkyl (hetero)cycloalkyl, or (hetero)aryl; R2 = (un)substituted (hetero)cycloalkyl, (hetero)aryl, ORd, NRcRd, or CO2Rd; R3 = (un)substituted (cyclo)alkyl, alkenyl, or alkynyl; R4 = H, ORc, CO2Rc, OCORc, OCO2Rc, OCONRdRe, NRdRe, NHCO2Rc, NRcSO2Rc, SO1-2Rc, or (un)substituted alkyl, alkenyl, alkynyl, or (hetero)aryl; R6 = H, halo, CN, NRcRd, or (un)substituted alkyl, alkenyl, or alkynyl; A = 3- to 8-membered (un)substituted monocyclic saturated ring incorporating the same C to which R4 is attached and optionally containing 1-2 heteroatoms, and to which a (hetero)aryl ring is fused, wherein said bicyclic ring is optionally fused to another (hetero)aryl ring to form a tricyclic ring; Rc and Rd = independently H or (un)substituted alkyl, alkenyl, alkynyl, (hetero)cycloalkyl(alkyl), or (hetero)aryl(alkyl); or NRcRd = (un)substituted heterocyclyl; or two ORc groups together with the atoms to which they are attached = (un)substituted heterocyclyl; Re = H, (cyclo)alkyl, alkenyl, alkynyl, (hetero)cycloalkyl(alkyl), or (hetero)aryl(alkyl); and pharmaceutically acceptable salts thereof] were prepared by conventional and automated synthesis methods as antagonists and/or inverse agonists of the cannabinoid-1 (CB1) receptor (no data). For example, 1,2,3,4-tetrahydro-2-naphthoic acid was converted to the acyl chloride using oxalyl chloride and DMF in CH2Cl2. Acylation of 2,3-bis(4-chlorophenyl)-1-methylpropylamine•HCl with the naphthoic chloride in the presence of diisopropylethylamine in CH2Cl2 provided a diastereomeric mixture of amides II, which were separated on a silica gel column. I and their pharmaceutical compns. are useful as psychotropic drugs in the treatment of psychosis, memory deficits, cognitive disorders, migraine, neuropathy, neuroinflammatory disorders, including multiple sclerosis and Guillain-Barre syndrome, and the inflammatory sequelae of viral encephalitis, cerebral vascular accidents, and head trauma, anxiety disorders, stress, epilepsy, Parkinson's disease, movement disorders, and schizophrenia (no data). In addition, I and their pharmaceutical compns. are useful for the treatment of substance abuse disorders, the treatment of obesity or eating disorders, as well as the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver (no data). Novel compds. of the structural formula (I) are antagonists and/or inverse agonists of the Cannabinoid-1 (CB1) receptor and are useful in the treatment, prevention and suppression of diseases mediated by the CB1 receptor.
- IT **92907-23-8P**, 3-(4-Chlorophenyl)-2-phenylpropanoic acid methyl ester  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; preparation of substituted bicyclic arylamide CB1 receptor antagonists and/or inverse agonists for use as psychotropic drugs)
- RN 92907-23-8 CAPLUS
- CN Benzenepropanoic acid, 4-chloro- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)

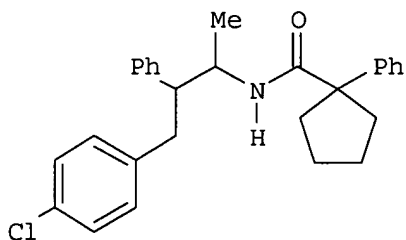




## CAS ONLINE PRINTOUT

TI Preparation of spirocyclic carboxamides as cannabinoid receptor modulators  
 IN Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.; Goulet, Mark T.;  
 Jewell, James P.  
 PA Merck & Co., Inc., USA  
 SO PCT Int. Appl., 224 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003082190	A2	20031009	WO 2003-US8722	20030321
	WO 2003082190	A3	20040219		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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	JP 2005528366	T2	20050922	JP 2003-579733	20030321
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PRAI	US 2002-367655P	P	20020326		
	WO 2003-US8722	W	20030321		
OS	MARPAT 139:307605				
GI					



AB R1CH2CR2R3CHR4NHCOA [R1 = (un)substituted alkyl, cycloalkyl, heterocyclic, aryl; R2 = (un)substituted cycloalkyl, heterocyclic, aryl, OH, NH2, CO2H; R3 = H, (un)substituted alkyl, alkenyl, alkynyl, OH, NH2, halogen, CN; R4 = H, (un)substituted alkyl; A = (un)substituted 3-8-membered carbocyclic ring] were prepared and are antagonists and/or inverse agonists of the cannabinoid-1 (CB1) receptor, useful as psychotropic drugs in the treatment of psychosis, memory deficits, cognitive disorders, migraine, neuropathy, neuro-inflammatory disorders including multiple sclerosis and Guillain-Barre syndrome and the inflammatory sequelae of viral encephalitis, cerebral vascular accidents, and head trauma, anxiety disorders, stress, epilepsy, Parkinson's disease, movement disorders, and schizophrenia. The compds. are also useful for the treatment of substance abuse disorders, the treatment of obesity or eating disorders, as well as, the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver. Thus, PhCH2CO2Me was

## CAS ONLINE PRINTOUT

treated with 4-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>Br to give 4-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CHPhCO<sub>2</sub>Me which was hydrolyzed to the acid, converted to 4-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CHPhCONMeOMe, and treated with MeMgBr to give 4-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CHPhCOMe. This ketone was reduced to the alc., converted to the mesylate and then to the azide which was reduced to 4-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CHPhCHMeNH<sub>2</sub>.HCl. Treatment of this amine with phenylcyclopentanecarboxylic acid gave the amide I.

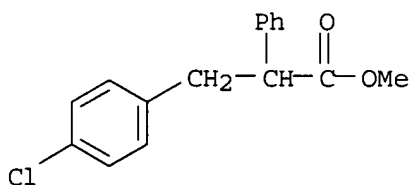
IT 92907-23-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of spirocyclic carboxamides as cannabinoid receptor modulators)

RN 92907-23-8 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 7 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:757469 CAPLUS

DN 139:276471

TI Preparation of substituted amides as antagonists and/or inverse agonists of the cannabinoid-1 receptor for therapy

IN Hagmann, William K.; Lin, Linus S.; Shah, Shrenik K.; Guthikonda, Ravindra N.; Qi, Hongbo; Chang, Linda L.; Liu, Ping; Armstrong, Helen M.; Jewell, James P.; Lanza, Thomas J., Jr.

PA Merck & Co., Inc., USA; et al.

SO PCT Int. Appl., 381 pp.

CODEN: PIXXD2

DT Patent

LA English

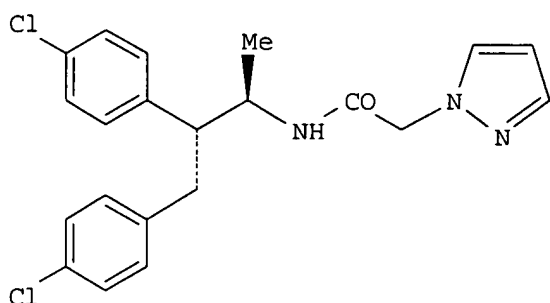
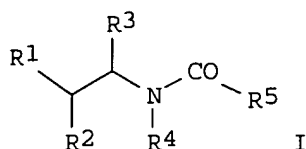
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003077847	A2	20030925	WO 2003-US7320	20030307
	WO 2003077847	A3	20041104		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2478183	AA	20030925	CA 2003-2478183	20030307
	EP 1496838	A2	20050119	EP 2003-714051	20030307
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2005519958	T2	20050707	JP 2003-575901	20030307
	US 2004058820	A1	20040325	US 2003-387265	20030312
	US 6972295	B2	20051206		
	US 2005234061	A1	20051020	US 2005-109076	20050419
PRAI	US 2002-363597P	P	20020312		

## CAS ONLINE PRINTOUT

US 2002-428351P	P	20021122
WO 2003-US7320	W	20030307
US 2003-387265	A3	20030312

OS MARPAT 139:276471  
GI



AB Novel compds. of the structural formula I (e.g. N-[2,3-bis(4-chlorophenyl)-1-methylpropyl]-2-(pyrazol-1-yl)acetamide trifluoroacetate (base shown as II with relative stereochem.); variables defined below) are antagonists and/or inverse agonists of the cannabinoid-1 (CB1) receptor (no data) and are useful in the treatment, prevention and suppression of diseases mediated by the CB1 receptor. The compds. of the present invention are useful as centrally acting drugs in the treatment of psychosis, memory deficits, cognitive disorders, migraine, neuropathy, neuro-inflammatory disorders including multiple sclerosis and Guillain-Barre syndrome and the inflammatory sequelae of viral encephalitis, cerebral vascular accidents, and head trauma, anxiety disorders, stress, epilepsy, Parkinson's disease, movement disorders, and schizophrenia. The compds. are also useful for the treatment of substance abuse disorders, the treatment of obesity or eating disorders, as well as the treatment of asthma, constipation, chronic intestinal pseudo-obstruction, and cirrhosis of the liver. Although the methods of preparation are not claimed, more than 120 example preps. of intermediates and >480 example preps./characterization data for a library of I are included. For I: R1 = C1-10-alkyl, C3-10cycloalkyl, C3-10-cycloalkyl-C1-4-alkyl, cycloheteroalkyl, cycloheteroalkyl-C1-4alkyl, aryl, aryl-C1-4-alkyl, heteroaryl, heteroaryl-C1-4-alkyl, -ORd, -NRcRd, -NRcC(O)Rd, -CO2Rd, and -C(O)NRcRd. R2 = C1-10alkyl, C3-10cycloalkyl-C1-4alkyl, cycloheteroalkyl, cycloheteroalkyl-C1-4alkyl, aryl, aryl-C1-4alkyl, aryloxy, arylthio, heteroaryl, and heteroaryl-C1-4alkyl; R3 = H, and C1-4alkyl; R4 = H, and C1-4alkyl; R5 = C1-10alkyl, C2-10alkenyl, C3-10-cycloalkyl-C1-4alkyl, cycloheteroalkyl-C1-4-alkyl, aryl-C1-4-alkyl, diaryl-C1-4alkyl, aryl-C1-4alkenyl, heteroaryl-C1-4alkyl, -ORd, and -NRcRd; addnl. details including provisos are given in the claims.

IT **92907-23-8P**, 3-(4-Chlorophenyl)-2-phenylpropanoic acid methyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

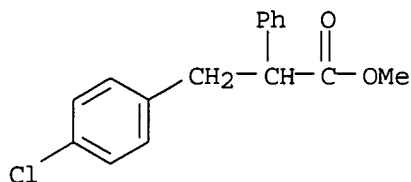
CAS ONLINE PRINTOUT

(Reactant or reagent)

(preparation of substituted amides as antagonists and/or inverse agonists of cannabinoid-1 receptor for therapy)

RN 92907-23-8 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 8 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:262921 CAPLUS

DN 139:85155

TI Intermolecular C-H activation at benzylic positions: synthesis of (+)-imperanene and (-)- $\alpha$ -conidendrin

AU Davies, Huw M. L.; Jin, Qihui

CS Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, NY, 14260-3000, USA

SO Tetrahedron: Asymmetry (2003), 14(7), 941-949

CODEN: TASYE3; ISSN: 0957-4166

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 139:85155

AB An efficient C-H activation of primary benzylic positions by means of rhodium carbenoid induced C-H insertions is described. This key step was used in concise syntheses of (+)-imperanene and (-)- $\alpha$ -conidendrin.

IT 553642-32-3

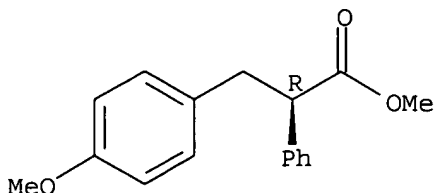
RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis of (+)-imperanene and (-)- $\alpha$ -conidendrin from a benzene derivative and a aryldiazoacetate via a rhodium carbenoid induced C-H insertion)

RN 553642-32-3 CAPLUS

CN Benzenepropanoic acid, 4-methoxy- $\alpha$ -phenyl-, methyl ester, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1999:9808 CAPLUS

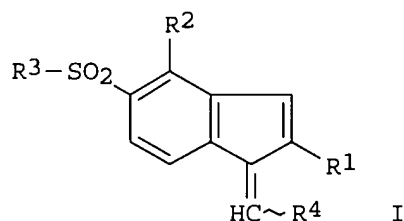
DN 130:81284

TI Preparation of indene derivatives as COX 2 inhibitors

## CAS ONLINE PRINTOUT

IN Matsuoka, Hiroharu; Maruyama, Noriaki; Kato, Yasuharu  
 PA Chugai Seiyaku Kabushiki Kaisha, Japan  
 SO PCT Int. Appl., 88 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9857924	A1	19981223	WO 1998-JP2611	19980615
	W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	JP 11071342	A2	19990316	JP 1998-163372	19980611
	AU 9876749	A1	19990104	AU 1998-76749	19980615
PRAI	JP 1997-159598	A	19970617		
	WO 1998-JP2611	W	19980615		
OS	MARPAT 130:81284				
GI					



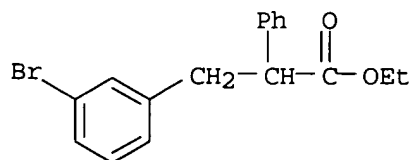
AB The title compds. I [R1 represents hydrogen etc.; R2 represents hydrogen etc.; R3 represents a C1-C3 linear or branched alkyl; and R4 represents an optionally substituted aryl etc.] are prepared The title compound (Z)-I [R1 = propyl; R2 = H; R3 = methyl; R4 = p-methoxyphenyl] in vitro showed IC50 values of 2  $\mu$ M and 8  $\mu$ M against COX-2 and COX-1, resp.

IT **218453-08-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of indene derivs. as COX 2 inhibitors)

RN 218453-08-8 CAPLUS

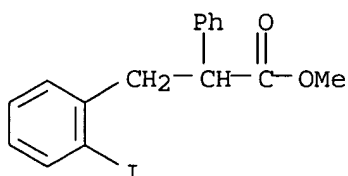
CN Benzenepropanoic acid, 3-bromo- $\alpha$ -phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

## CAS ONLINE PRINTOUT

L13 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1998:785207 CAPLUS  
DN 130:252002  
TI Sandmeyer reactions. Part 4. An investigation into the cyclization modes of Pschorr phenanthrene synthesis  
AU Hanson, Peter; Lovenich, P. Wilfried; Rowell, Simon C.; Walton, Paul H.; Timms, Allan W.  
CS Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK  
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1999), (1), 49-64  
CODEN: JCPKBH; ISSN: 0300-9580  
PB Royal Society of Chemistry  
DT Journal  
LA English  
AB Comparison of the cyclization regiochem. of the heterolysis and Cu-catalyzed homolysis of Me (E)-3-(2-diazoniophenyl)-2-(3-halophenyl)propenoate tetrafluoroborates indicates that the homolytic pathway involves direct closure of the 5-membered ring and not a 5-membered ring closure followed by ring expansion. From competition expts. in which homolytic cyclization of the corresponding non-halogenated compound was run against H abstraction from H3PO2, a cyclization rate constant  $k_C = (3.0 \pm 0.5) \times 10^9 \text{ s}^{-1}$  at ambient temperature was estimated which, when used in conjunction with a literature value for the homolytic phenylation of C6H6, allows evaluation of a statistically corrected effective molarity of  $2 \times 10^4 \text{ mol dm}^{-3}$  for homolytic Pschorr phenanthrene closure. Regioselectivity considerations imply that, by contrast, heterolytic Pschorr phenanthrene closure exhibits unit effective molarity. A mechanistic rationale is presented to explain these patterns of behavior.  
IT **221466-89-3P**  
RL: BYP (Byproduct); PREP (Preparation)  
(mechanism of Sandmeyer reaction in Pschorr phenanthrene synthesis)  
RN 221466-89-3 CAPLUS  
CN Benzenepropanoic acid, 2-iodo- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1998:23032 CAPLUS  
DN 128:127797  
TI Diastereoselective reactions of 1,1'-binaphthyl ester enolates with carbonyl electrophiles  
AU Ahn, Mija; Tanaka, Kiyoshi; Fuji, Kaoru  
CS Institute for Chemical Research, Kyoto University, Kyoto, 611, Japan  
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (2), 185-192  
CODEN: JCPRB4; ISSN: 0300-922X  
PB Royal Society of Chemistry  
DT Journal  
LA English

## CAS ONLINE PRINTOUT

OS CASREACT 128:127797

AB Diastereoselectivity in the aldol and the conjugate addns. of 2'-hydroxy-1,1'-binaphthyl ester enolates with a variety of carbonyl electrophiles has been examined. The ester enolate generated by BuLi reacts with several aldehydes to give the threo products preferentially with high diastereoselectivity and in good yield. Satisfactory diastereoselectivity has also been observed in the minor erythro derivs. A mechanistic interpretation of the results is made on the basis of the absolute stereochem. of the products.

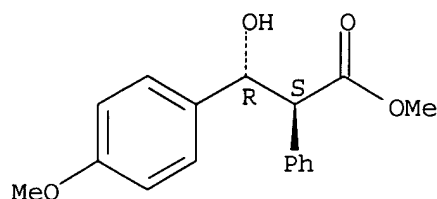
IT 201746-39-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(diastereoselective reactions of 1,1'-binaphthyl ester enolates with carbonyl electrophiles)

RN 201746-39-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methoxy- $\alpha$ -phenyl-, methyl ester, [R-(R\*,S\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 12 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:280921 CAPLUS

DN 126:277281

TI Preparation of N-(2,3-diphenyl-2-propenoyl)guanidine derivatives as inhibitors of sodium/proton exchanger

IN Okazaki, Toshio; Kikuchi, Kazumi; Toyoshima, Hiroshi; Takanashi, Masahiro; Yanagisawa, Isao

PA Yamanouchi Pharma Co Ltd, Japan

SO Jpn. Kokai Tokkyo Koho, 14 pp.

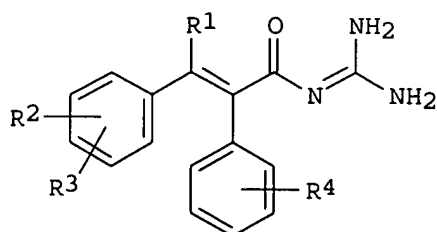
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 09059245	A2	19970304	JP 1995-217869	19950825
PRAI	JP 1995-217869		19950825		
OS	MARPAT 126:277281				
GI					



CAS ONLINE PRINTOUT

AB The title compds. [I; R1 = H, halo, lower alkyl; R2, R3, R4 = H, lower (halo)alkyl, lower alkenyl, lower alkynyl, cycloalkyl, lower alkoxy, lower alkoxy-lower alkyl, lower alkoxy-carbonyl, CO<sub>2</sub>H, halo, NO<sub>2</sub>, cyano, NH<sub>2</sub>, mono- or di(lower alkyl)amino, lower alkanoyl, lower alkanoylamino, lower alkanoyloxy, OH, SH, lower alkylthio, lower alkylsulfonyl, mono- or di(lower alkyl)aminosulfonyl, etc.], which are useful for the treatment of hypertension, arrhythmia, and angina pectoris or as diagnostic agents for Na<sup>+</sup>/H<sup>+</sup> exchanger-related hypertension, diabetes, and arteriosclerosis (no data), are prepared. Thus, a mixture of 0.90 g (E)-3-(m-methoxyphenyl)-2-phenyl-2-propenoic acid (preparation given), 0.57 g 1,1'-carbonylbis(1H-imidazole), and 12 mL DMF was stirred at 50° for 30 min and ice-cooled, to which a solution of guanidine in DMF (preparation given), and the resulting mixture was stirred at room temperature for 3 h to give I (R1 = R3 = R4 = H, R2 = 3-MeO).

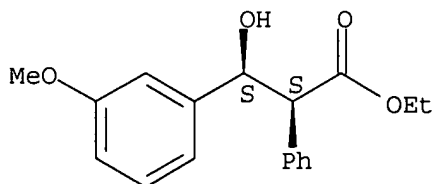
IT 188752-93-4P 188752-94-5P 188752-97-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of N-(diphenylpropenoyl)guanidine derivs. as inhibitors of sodium/proton exchanger)

RN 188752-93-4 CAPLUS

CN Benzenepropanoic acid, β-hydroxy-3-methoxy-α-phenyl-, ethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

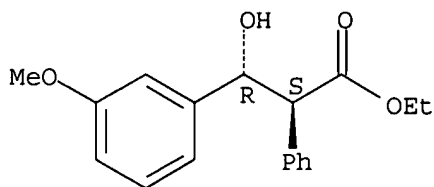
Relative stereochemistry.



RN 188752-94-5 CAPLUS

CN Benzenepropanoic acid, β-hydroxy-3-methoxy-α-phenyl-, ethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

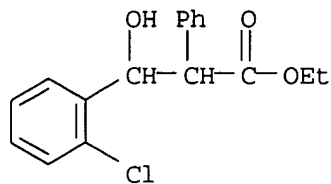


RN 188752-97-8 CAPLUS

CN Benzenepropanoic acid, 2-chloro-β-hydroxy-α-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



## CAS ONLINE PRINTOUT



L13 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:656165 CAPLUS

DN 115:256165

TI Preparation of N-benzylated imidazopyridines and benzimidazoles as  
angiotensin II antagonistsIN Greenlee, William J.; Patchett, Arthur A.; Hangauer, David; Walsh, Thomas;  
Fitch, Kenneth J.; Rivero, Ralph A.; Dhanoa, Daljit S.

PA Merck and Co., Inc., USA

SO PCT Int. Appl., 401 pp.

CODEN: PIXXD2

DT Patent

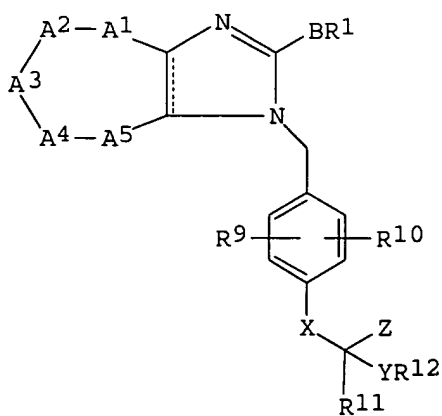
LA English

FAN.CNT 2

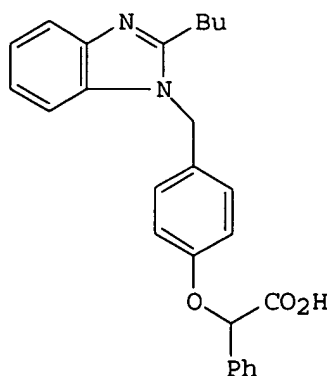
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9111999	A1	19910822	WO 1991-US957	19910211
	W: CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
	CA 2075627	AA	19910814	CA 1991-2075627	19910211
	CA 2075637	AA	19910814	CA 1991-2075637	19910211
	EP 517812	A1	19921216	EP 1991-905733	19910211
	R: CH, DE, FR, GB, IT, LI, NL				
	JP 05504969	T2	19930729	JP 1991-505964	19910211
	US 5240938	A	19930831	US 1991-744557	19910813
	US 5264439	A	19931123	US 1991-744138	19910813
	US 5449682	A	19950912	US 1993-61975	19930517
PRAI	US 1990-479786	A	19900213		
	WO 1991-US957	W	19910211		
	US 1991-671551	B2	19910319		
	US 1991-671552	B2	19910319		
	US 1991-744557	A3	19910813		

OS MARPAT 115:256165

GI



I



II

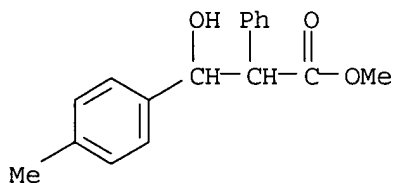
AB Title compds. [I; R1 = (substituted) alkyl, alkenyl, alkynyl, (hetero)aryl, perfluoroalkyl; R9, R10 = H, (cycloalkyl)alkyl, alkenyl, alkynyl, halo, alkoxy, perfluoroalkyl, (alkyl)cycloalkyl, aryl; adjacent R9R10 = CH:CHCH:CH; R11, R12 = H, (substituted) alkyl, aryl, arylalkyl, cycloalkyl; B = bond, SOn(CH2)s, O; n = 0-2; s = 0-5; X = O, SOn, imino, CH2O, CH2, CH2CH2, bond SOnCH2, etc.; Y = bond, SOn imino, CH2; Z = CO2H, alkoxy carbonyl, tetrazol-5-yl, arylsulfonylcarbamoyl, P(O)(OH)2, etc.; A1-A2-A3-A4-A5 = moieties to complete (substituted) benzene or heterocyclic (e.g., pyridine) rings], were prepared as antihypertensives, nootropics, anxiolytics, and antidepressants (no data). Thus, 2-butylbenzimidazole and 4-(PhCH2O)C6H4Cl were condensed to give 96% N-benzylated product, which was hydrogenolyzed (83%) followed by condensation with BrCHPhCO2Me (17%) and saponification (30%) to give title compound II.

IT **137420-61-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as intermediate for angiotensin II antagonist)

RN 137420-61-2 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methyl- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 14 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1990:198049 CAPLUS

DN 112:198049

TI Preparation of some chromans substituted at the 3- or 4-position by an aryl or benzyl group by the rhodium-catalyzed intramolecular nucleophilic substitution of the corresponding 3-(2-fluorophenyl)propan-1-ols

AU Houghton, Roy P.; Shervington, Leroy A.

CS Coll. Cardiff, Univ. Wales, Cardiff, CF1 3TB, UK

SO Journal of Chemical Research, Synopses (1989), (8), 239

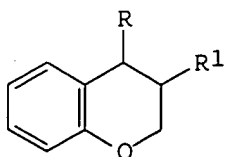
CODEN: JRPSDC; ISSN: 0308-2342

DT Journal

LA English

OS CASREACT 112:198049

GI



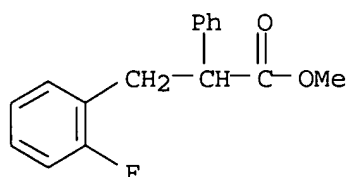
I

AB [Rh( $\eta^5$ -C<sub>5</sub>EtMe<sub>4</sub>)( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>)] [PF<sub>6</sub>]<sub>2</sub> catalyzed the formation of chromans (I; R = H, CH<sub>2</sub>OH, Ph, 2-FC<sub>6</sub>H<sub>4</sub>, CH<sub>2</sub>Ph; R<sub>1</sub> = Ph, 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 4-MeOC<sub>6</sub>H<sub>4</sub>, CH<sub>2</sub>OH, H) from 2-FC<sub>6</sub>H<sub>4</sub>CHRCHR<sub>1</sub>CH<sub>2</sub>OH in MeNO<sub>2</sub>-Me<sub>2</sub>CO.

IT **126348-02-5P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reduction of)

RN 126348-02-5 CAPLUS

CN Benzenepropanoic acid, 2-fluoro- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 15 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:630289 CAPLUS

DN 101:230289

TI Studies on antifertility agents: part XLII - synthesis and antifertility study of 6-methoxy-3-phenyl-1-[p-( $\beta$ -pyrrolidinoethoxy)phenyl]tetralin

AU Malik, Mangel S.; Rastogi, Shri Nivas

CS Med. Chem. Div., Cent. Drug Res. Inst., Lucknow, 226 001, India

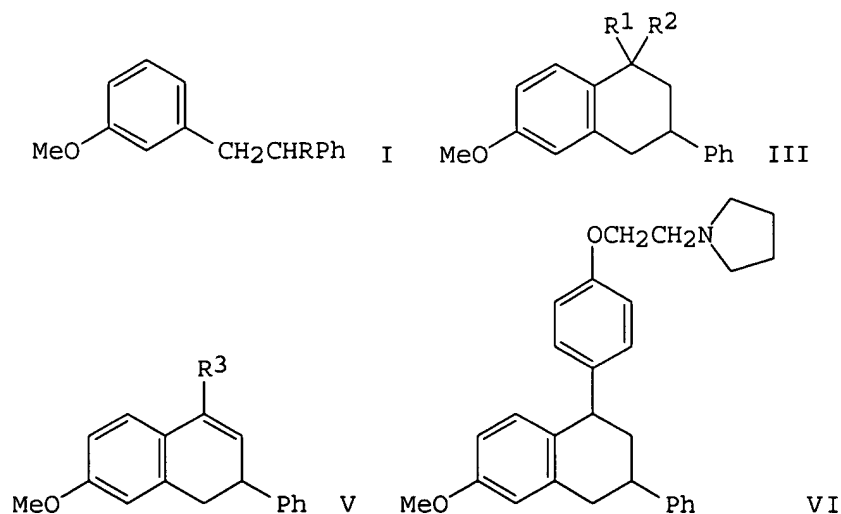
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(9), 834-8  
 CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

OS CASREACT 101:230289

GI



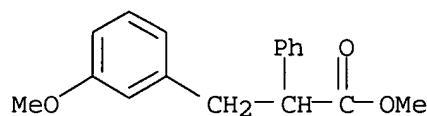
## CAS ONLINE PRINTOUT

AB LiAlH<sub>4</sub> reduction of ester I (R = MeO<sub>2</sub>C) gave the propanol I (R = HOCH<sub>2</sub>), which after treatment with p-TsCl and KCN gave butyronitrile I (R = NCCH<sub>2</sub>) (II). Alkaline hydrolysis of II gave acid I (R = HO<sub>2</sub>CCH<sub>2</sub>), which was cyclized on PCl<sub>5</sub>-SnCl<sub>4</sub> to give tetralone derivative (III; R<sub>1</sub>R<sub>2</sub> = O) (IV). KBH<sub>4</sub> reduction of IV gave predominantly cis-tetrol (III; R<sub>1</sub> = H, R<sub>2</sub> = HO), which was condensed with PhOH-AlCl<sub>3</sub> to give cis- and trans-III (R<sub>1</sub> = H, R<sub>2</sub> = 2- and 4-HOC<sub>6</sub>H<sub>4</sub>), and V (R<sub>3</sub> = H). Reaction of Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>MgCl with tetralone IV gave the propylamine V (R<sub>3</sub> = Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>). Condensation of III (R<sub>1</sub> = H, R<sub>2</sub> = 4-HOC<sub>6</sub>H<sub>4</sub>) with N-(2-chloroethyl)pyrrolidine gave the title compound (VI).

IT **93273-50-8P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reduction of)

RN 93273-50-8 CAPLUS

CN Benzenepropanoic acid, 3-methoxy- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 16 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:209410 CAPLUS

DN 100:209410

TI  $\beta$ -Hydroxy esters

PA Mitsui Petrochemical Industries, Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 59013748	A2	19840124	JP 1982-123020	19820716
PRAI	JP 1982-123020		19820716		

AB Ten  $\beta$ -hydroxy esters were prepared by reaction of  $\alpha$ -halo esters with Sn and carbonyl compds. in a polar solvent, followed by hydrolysis. Thus, PhCHBrCO<sub>2</sub>Et 243 and PhCHO 85 were added to Sn 131 mg in DMF at -45°, the mixture stirred overnight at -45°, and H<sub>2</sub>O added to give 78% HOCHPhCHPhCO<sub>2</sub>Et (84:16 erythro-threo).

IT **81807-53-6P 81807-54-7P 81807-55-8P**

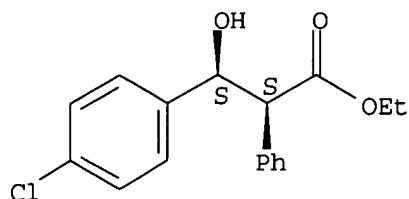
**81807-56-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 81807-53-6 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, ethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

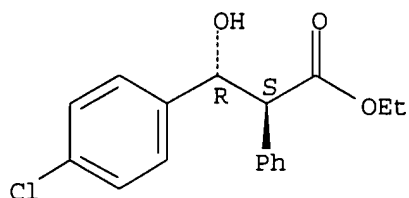
Relative stereochemistry.



RN 81807-54-7 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, ethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

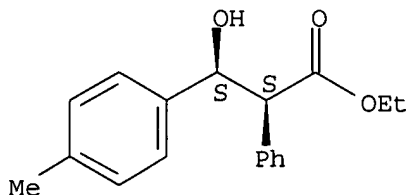
Relative stereochemistry.



RN 81807-55-8 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methyl- $\alpha$ -phenyl-, ethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

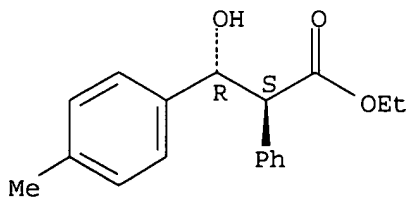
Relative stereochemistry.



RN 81807-56-9 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methyl- $\alpha$ -phenyl-, ethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 17 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1982:581388 CAPLUS

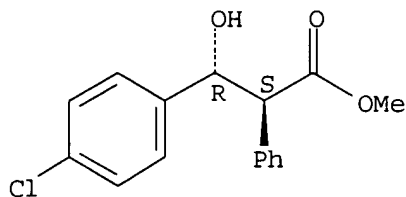
DN 97:181388

TI Dehydrative decarboxylation of 2,3-disubstituted 3-hydroxycarboxylic acids with dimethylformamide acetals - apparent reaction course and preparative possibilities

## CAS ONLINE PRINTOUT

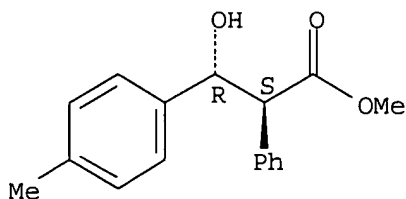
AU Mulzer, Johann; Bruentrup, Gisela  
CS Inst. Org. Chem., Univ. Muenchen, Munich, D-8000/2, Fed. Rep. Ger.  
SO Chemische Berichte (1982), 115(6), 2057-75  
CODEN: CHBEAM; ISSN: 0009-2940  
DT Journal  
LA German  
OS CASREACT 97:181388  
AB Me<sub>2</sub>NCH(OMe)<sub>2</sub> (I) converted threo-RCH(OH)CHR<sub>1</sub>CO<sub>2</sub>H (II; R = H, alkyl, vinyl, styryl, Ph, substituted Ph, 2-furyl, 2-thienyl; R<sub>1</sub> = Me, Et, CHMe<sub>2</sub>, CMe<sub>3</sub>, Ph) to (E)- (III)/(Z)-RCH:CHR<sub>1</sub> mixts. only when R = aryl or vinyl. The reaction had a marked E selectivity but was not a stereo-controlled olefin synthesis. If R = alkyl, the Me esters of II were obtained in the reaction. I reacted with erythro-II to give >98% sterically pure III. The fragmentation of zwitterionic intermediates was discussed.  
IT **55006-65-0P 60079-78-9P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 55006-65-0 CAPLUS  
CN Benzenepropanoic acid, 4-chloro-β-hydroxy-α-phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 60079-78-9 CAPLUS  
CN Benzenepropanoic acid, β-hydroxy-4-methyl-α-phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 18 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1982:217397 CAPLUS  
DN 96:217397  
TI A new method for the synthesis of β-hydroxy esters by using metallic tin  
AU Harada, Taira; Mukaiyama, Teruaki  
CS Fac. Sci., Univ. Tokyo, Tokyo, 113, Japan  
SO Chemistry Letters (1982), (2), 161-4  
CODEN: CMLTAG; ISSN: 0366-7022  
DT Journal  
LA English  
OS CASREACT 96:217397  
AB Metallic Sn or activated metallic Sn, prepared by reduction of SnCl<sub>2</sub> with

CAS ONLINE PRINTOUT

LiAlH<sub>4</sub>, smoothly reacts with  $\alpha$ -halo esters to yield the Sn enolates, which in turn react with carbonyl compds. under mild conditions to give, after hydrolysis,  $\beta$ -hydroxy esters in high yields.

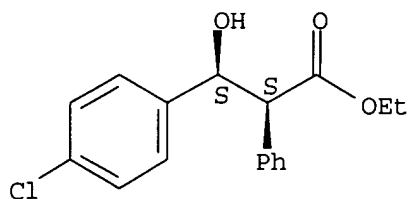
IT 81807-53-6P 81807-54-7P 81807-55-8P  
81807-56-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 81807-53-6 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, ethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

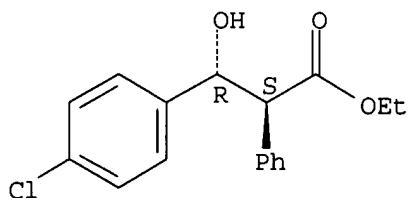
Relative stereochemistry.



RN 81807-54-7 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, ethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

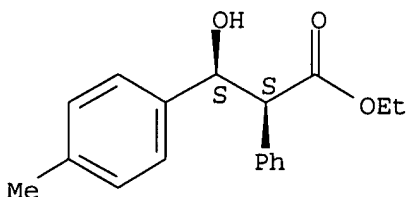
Relative stereochemistry.



RN 81807-55-8 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methyl- $\alpha$ -phenyl-, ethyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

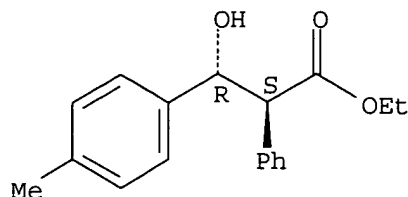
Relative stereochemistry.



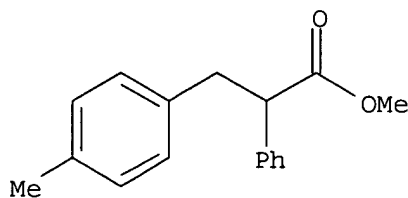
RN 81807-56-9 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methyl- $\alpha$ -phenyl-, ethyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 19 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1979:419169 CAPLUS  
 DN 91:19169  
 TI Catalytic transfer reduction: scope and utility  
 AU Brieger, Gottfried; Nestricks, Terry J.; Fu, Tzuu-Heng  
 CS Dep. Chem., Oakland Univ., Rochester, MI, USA  
 SO Journal of Organic Chemistry (1979), 44(11), 1876-8  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DT Journal  
 LA English  
 AB The Pd-catalyzed H transfer from organic donors to olefins, aromatic aldehydes, and ketones was studied. The intermediate benzyl alc. formed in the reduction of aromatic aldehydes can be trapped as the corresponding acetate. In the reduction of more complex ketones, ring opening occurs with cyclopropanes, and hydrogenolysis of aromatic halides also occurs. The relative effectiveness of a variety of donor compds. is also reported. Asym. induction during catalytic H transfer was explored with several systems, but no evidence of optical activity was found.  
 IT **69668-17-3P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 69668-17-3 CAPLUS  
 CN Benzenepropanoic acid, 4-methyl- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 20 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1978:529206 CAPLUS  
 DN 89:129206  
 TI Interaction of substituted benzaldehydes with methylphenylacetate during low-temperature Claisen reaction  
 AU Kirchev, N.; Krachanov, Kh.  
 CS Inst. Food Technol., Plovdiv, Bulg.  
 SO Doklady Bolgarskoi Akademii Nauk (1978), 31(1), 59-61  
 CODEN: DBANAD; ISSN: 0366-8681  
 DT Journal  
 LA English  
 AB Reaction of  $\text{PhCH}_2\text{CO}_2\text{Me}$  with  $\text{RnC}_6\text{H}_5\text{-nCHO}$  ( $\text{Rn} = \text{H}, 2\text{-F}, 2\text{-Cl}, 3\text{-Cl}, 2,6\text{-Cl}_2, 3\text{-Me}, 4\text{-MeO}$ , etc.) in  $\text{Et}_2\text{O}$  at  $-24^\circ$  for 2 h in the presence of  $\text{NaNH}_2$  stopped at the aldol stage and gave eighteen  $\text{RnC}_6\text{H}_5\text{-nCH(OH)CHPhCO}_2\text{Me}$  (I) in 31-85% yield, with threo/erythro ratio in the product varying from 96:4



CAS ONLINE PRINTOUT

to 69:31. There was no well-defined relation between the nature and position of the substituent and the yield of I.

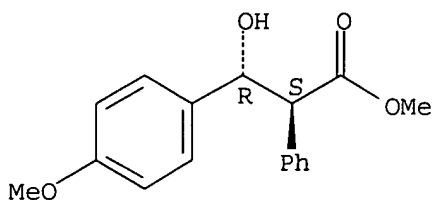
IT 20445-41-4P 55006-62-7P 55006-63-8P  
 55006-64-9P 55006-65-0P 55006-67-2P  
 55006-68-3P 60079-78-9P 60079-81-4P  
 67710-01-4P 67710-04-7P 67710-05-8P  
 67710-06-9P 67722-11-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 20445-41-4 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methoxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

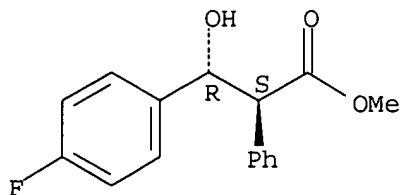
Relative stereochemistry.



RN 55006-62-7 CAPLUS

CN Benzenepropanoic acid, 4-fluoro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

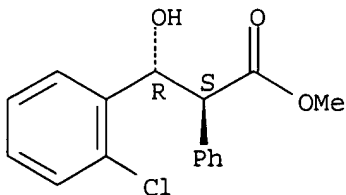
Relative stereochemistry.



RN 55006-63-8 CAPLUS

CN Benzenepropanoic acid, 2-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

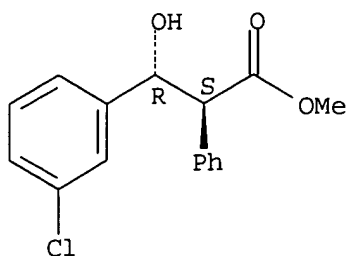


RN 55006-64-9 CAPLUS

CN Benzenepropanoic acid, 3-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

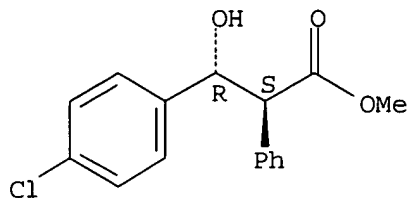
CAS ONLINE PRINTOUT



RN 55006-65-0 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

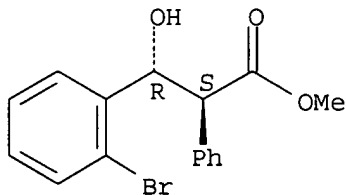
Relative stereochemistry.



RN 55006-67-2 CAPLUS

CN Benzenepropanoic acid, 2-bromo- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

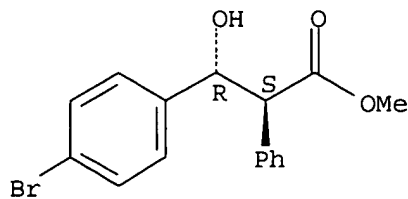
Relative stereochemistry.



RN 55006-68-3 CAPLUS

CN Benzenepropanoic acid, 4-bromo- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

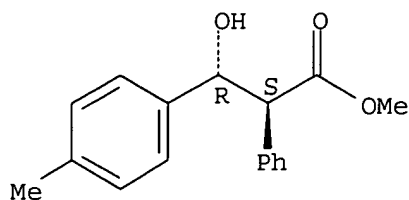


RN 60079-78-9 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methyl- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

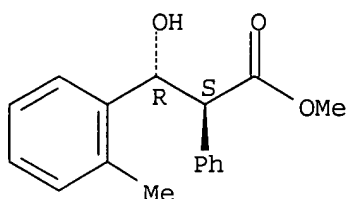
CAS ONLINE PRINTOUT



RN 60079-81-4 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-2-methyl- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

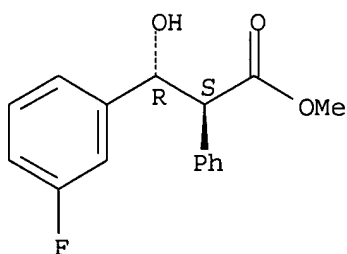
Relative stereochemistry.



RN 67710-01-4 CAPLUS

CN Benzenepropanoic acid, 3-fluoro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

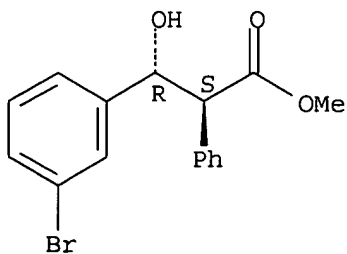
Relative stereochemistry.



RN 67710-04-7 CAPLUS

CN Benzenepropanoic acid, 3-bromo- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



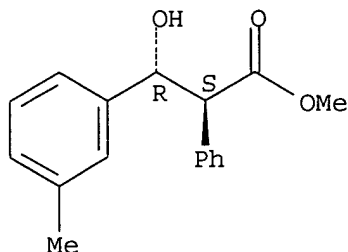
RN 67710-05-8 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-3-methyl- $\alpha$ -phenyl-, methyl

CAS ONLINE PRINTOUT

ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

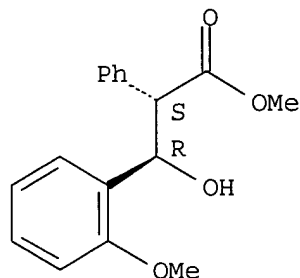
Relative stereochemistry.



RN 67710-06-9 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-2-methoxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

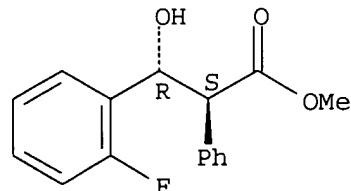
Relative stereochemistry.



RN 67722-11-6 CAPLUS

CN Benzenepropanoic acid, 2-fluoro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 21 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1977:72650 CAPLUS

DN 86:72650

TI 1-( $\beta$ -Aryl- $\beta$ -R-ethyl)imidazoles as antimicrobial agents

IN Heeres, Jan; Backx, Leo J. J.; Mostmans, Joseph H.

PA Janssen Pharmaceutica N. V., Belg.

SO U.S., 18 pp. Division of U.S. 3,927,017.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

PATENT NO.

KIND

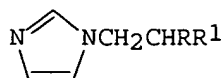
DATE

APPLICATION NO.

DATE

## CAS ONLINE PRINTOUT

PI	US 3991201	A	19761109	US 1975-578777	19750519
	US 3927017	A	19751216	US 1974-483587	19740627
PRAI	US 1974-483587	A3	19740627		
GI					



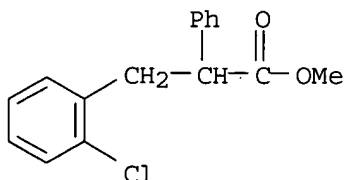
I

AB Arylethylimidazoles I (R = 4-FC6H4, 4-ClC6H4, 2-ClC6H4, 2,4-Cl2C6H3, 2,6-Cl2C6H3, Ph; R1 = C1-8 alkyl, allyl, 2-ClC6H4CH:CHCH2, chlorobenzyl, bromobenzyl, cyclohexyl, cyclopentyl, 4-MeOC6H4CH2, 4-MeC6H4CH2) (55 compds.) were prepared by treating RCH2CN with R1Br, hydrolyzing RR1CHCN, esterifying RR1CHCO2H, LiBH4 reduction of RR1CHCO2Me, treatment of RR1CHCH2OH with MeSO3H, and treatment of RR1CHCH2O3SMe with imidazole.

IT **59667-05-9P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 59667-05-9 CAPLUS

CN Benzenepropanoic acid, 2-chloro- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 22 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1976:477455 CAPLUS

DN 85:77455

TI Effect of substituents on the stereochemistry of the Reformatskii reaction

AU Mladenova, M.; Blagoev, B.; Kurtev, B.

CS Inst. Org. Chem., Sofia, Bulg.

SO Doklady Bolgarskoi Akademii Nauk (1975), 28(12), 1633-6  
 CODEN: DBANAD; ISSN: 0366-8681

DT Journal

LA French

AB The Reformatskii reaction of RC6H4CHO (R = H, p-Me, o-Me, p-Cl, o-Cl, p-MeO) and 1-naphthaldehyde with p-R1C6H4CHBrCO2Me (R1 = Br, H) gave an .apprx.50:50 mixture of erythro- and threo-RC6H4CH(OH)CH(C6H4R1-p)CO2Me or the 1-naphthyl analog in Et2O. In (MeO)2CH2, the erythro isomer was slightly favored (.apprx.60:40); in Me2SO, the threo isomer was favored (.apprx.70:30). In Me2SO, p-R1C6H4CH(CO2Me)CH(CO2Me)C6H4R-p was also formed. The lack of substituent effects in the Reformatskii reaction was explained by a transition state resembling the starting materials.

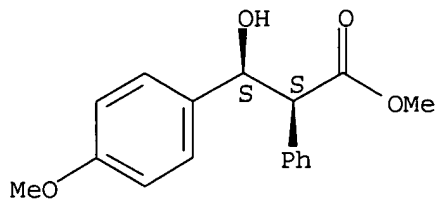
IT **20414-14-6P 20445-41-4P 55006-63-8P**  
**55006-65-0P 60079-78-9P 60079-79-0P**  
**60079-80-3P 60079-81-4P 60079-82-5P**  
**60079-83-6P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 20414-14-6 CAPLUS

CAS ONLINE PRINTOUT

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methoxy- $\alpha$ -phenyl-, methyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

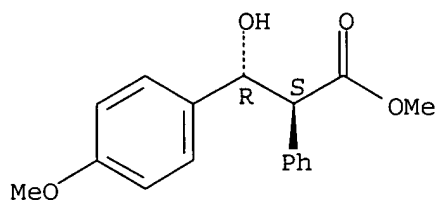
Relative stereochemistry.



RN 20445-41-4 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methoxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

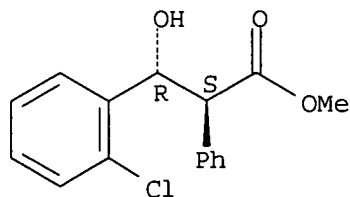
Relative stereochemistry.



RN 55006-63-8 CAPLUS

CN Benzenepropanoic acid, 2-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

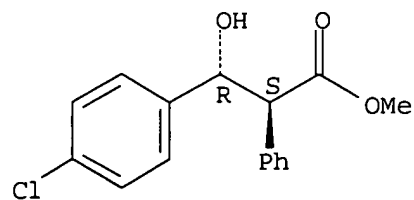
Relative stereochemistry.



RN 55006-65-0 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



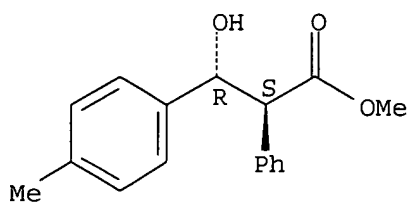
RN 60079-78-9 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methyl- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

CAS ONLINE PRINTOUT

ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

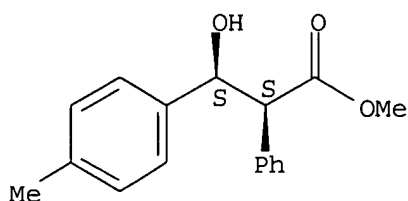
Relative stereochemistry.



RN 60079-79-0 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methyl- $\alpha$ -phenyl-, methyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

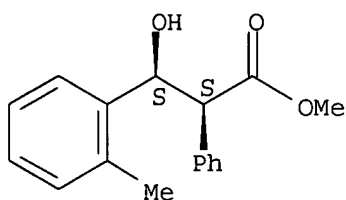
Relative stereochemistry.



RN 60079-80-3 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-2-methyl- $\alpha$ -phenyl-, methyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

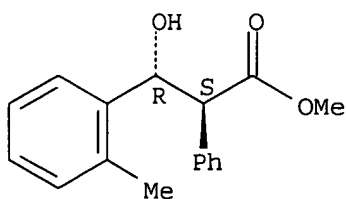
Relative stereochemistry.



RN 60079-81-4 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-2-methyl- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

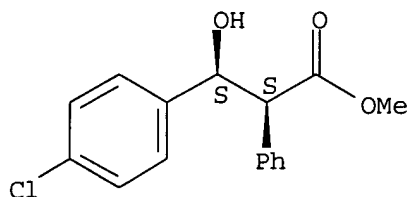
Relative stereochemistry.



RN 60079-82-5 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

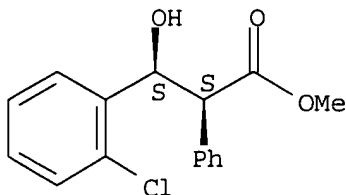
Relative stereochemistry.



RN 60079-83-6 CAPLUS

CN Benzenepropanoic acid, 2-chloro-β-hydroxy-α-phenyl-, methyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 23 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1976:433007 CAPLUS

DN 85:33007

TI 1-(β-Aryl-β-R-ethyl)imidazoles

IN Heeres, Jan; Backx, Leo J. J.; Mostmans, Joseph H.

PA Janssen Pharmaceutica N. V., Belg.

SO U.S., 16 pp.

CODEN: USXXAM

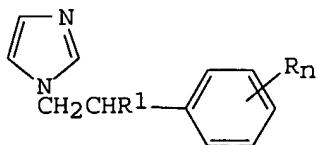
DT Patent

LA English

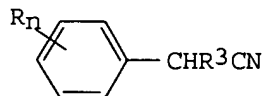
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	---	----	-----	-----
PI	US 3927017	A	19751216	US 1974-483587	19740627
	US 3991201	A	19761109	US 1975-578777	19750519
PRAI	US 1974-483587	A3	19740627		

GI



I



II

AB Imidazoles I [ $R_n = \text{Cl}, \text{F}, \text{H}, 2,4\text{-}, 2,6\text{-Cl}_2$ ;  $R_1 = \text{alkyl}, \text{allyl}, \text{cycloalkyl}, \text{CH}_2\text{C}_6\text{H}_5, \text{CH}_2\text{C}_6\text{H}_4\text{Cl}_2\text{-}2,4, \text{CH}_2\text{C}_6\text{H}_4\text{Cl}_2\text{-}2,6$ ;  $R_2 = \text{Cl}, \text{Br}, 4\text{-Me}, 4\text{-MeO}, \text{CH}_2\text{CH}_2\text{Ph}$ ] (53 compds.), fungicides, bacteriostats, and bactericides at 0.1-100  $\gamma/\text{ml}$ , were prepared by treating benzeneacetonitriles II ( $R_3 = \text{H}$ ) with halides  $R_1\text{X}$ , hydrolyzing-esterifying II ( $R_3 = R_1$ ) with  $\text{HCl}$  in  $\text{MeOH}$  or  $\text{EtOH}$ , reducing the ester  $R_n\text{C}_6\text{H}_5\text{-nCHR}_1\text{CO}_2\text{R}_4$  ( $R_4 = \text{Me}, \text{Et}$ ) with  $\text{NaBH}_4$



## CAS ONLINE PRINTOUT

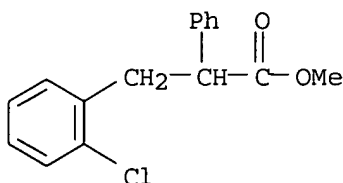
over LiX in MeCN, mesylating the alc.  $\text{RnC}_6\text{H}_5\text{-nCHRICH}_2\text{OH}$ , and treating the methanesulfonate with imidazole.

IT **59667-05-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 59667-05-9 CAPLUS

CN Benzenepropanoic acid, 2-chloro- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 24 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1975:125008 CAPLUS

DN 82:125008

TI Application of the low temperature Claisen reaction for stereoselective synthesis of threo-3-aryl-3-hydroxy-2-phenylpropanoic acids and their methyl esters

AU Kurtev, B.; Kratchanov, Kh.; Kirchev, N.

CS Inst. Org. Chem., Sofia, Bulg.

SO Synthesis (1975), (2), 106-8

CODEN: SYNTBF; ISSN: 0039-7881

DT Journal

LA English

OS CASREACT 82:125008

AB  $\text{RCHO}$  ( $\text{R} = \text{Ph}$ , 4- $\text{FC}_6\text{H}_4$ , 2-, 3-, 4- $\text{ClC}_6\text{H}_4$ , 2,6- $\text{Cl}_2\text{C}_6\text{H}_3$ , 2- and 4- $\text{BrC}_6\text{H}_4$ ) condensed with  $\text{PhCH}_2\text{CO}_2\text{R}_1$  ( $\text{R}_1 = \text{Me}$ ,  $\text{CMe}_3$ ) at  $-24^\circ$  in  $\text{Et}_2\text{O}$  or  $(\text{Me}_2\text{CH})_2\text{O}$  containing  $\text{NaNH}_2$  gave threo- $\text{HOCHRCHPhCO}_2\text{R}_1$  (I) in 40-85% yield from the solid phase of the reaction mixture; I ( $\text{R} = \text{Ph}$ ,  $\text{R}_1 = \text{CMe}_3$ ) was hydrolyzed to I ( $\text{R} = \text{Ph}$ ,  $\text{R}_1 = \text{H}$ ) in 93% yield by heating with  $\text{CF}_3\text{CO}_2\text{H}$ . The I yield was lower and the erythro-threo ratio was higher in different solvents or with  $\text{NaOEt}$  instead of  $\text{NaNH}_2$ .

IT **55006-62-7P 55006-63-8P 55006-64-9P**

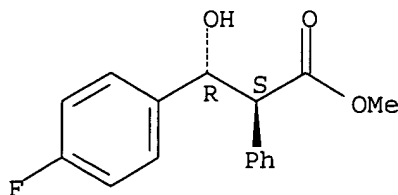
**55006-65-0P 55006-67-2P 55006-68-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 55006-62-7 CAPLUS

CN Benzenepropanoic acid, 4-fluoro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, ( $\text{R}^*$ , $\text{S}^*$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.

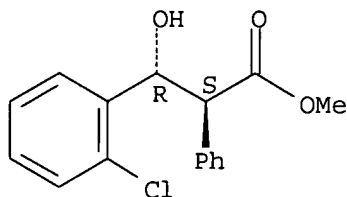


RN 55006-63-8 CAPLUS

CN Benzenepropanoic acid, 2-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, ( $\text{R}^*$ , $\text{S}^*$ )- (9CI) (CA INDEX NAME)

CAS ONLINE PRINTOUT

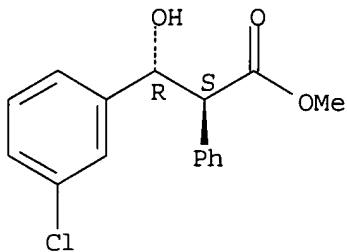
Relative stereochemistry.



RN 55006-64-9 CAPLUS

CN Benzenepropanoic acid, 3-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

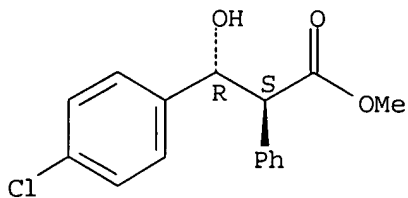
Relative stereochemistry.



RN 55006-65-0 CAPLUS

CN Benzenepropanoic acid, 4-chloro- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

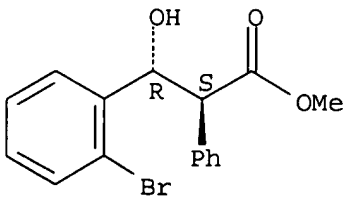
Relative stereochemistry.



RN 55006-67-2 CAPLUS

CN Benzenepropanoic acid, 2-bromo- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



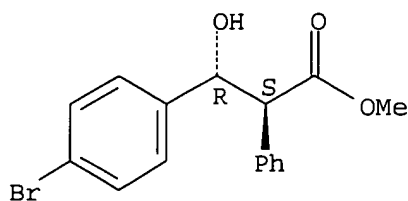
RN 55006-68-3 CAPLUS

CN Benzenepropanoic acid, 4-bromo- $\beta$ -hydroxy- $\alpha$ -phenyl-, methyl

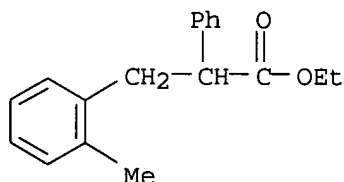
CAS ONLINE PRINTOUT

ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 25 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1974:477571 CAPLUS  
 DN 81:77571  
 TI Regiospecificity of methylation of unsymmetrical stilbenes by  
 (methylsulfinyl)methanide  
 AU James, Brian G.; Pattenden, Gerald  
 CS Dep. Chem., Univ. Coll., Cardiff, UK  
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and  
 Bio-Organic Chemistry (1972-1999) (1974), (10), 1195-204  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DT Journal  
 LA English  
 AB (E)-2-MeC<sub>6</sub>H<sub>4</sub>CH:CHPh with MeS(O)C-H<sub>2</sub> for 2 min gave .apprx.50%  
 (E)-2-MeC<sub>6</sub>H<sub>4</sub>CH:CMPh (I) and 2-MeC<sub>6</sub>H<sub>4</sub>CH [CH<sub>2</sub>S(O)Me]CH<sub>2</sub>Ph (II). Reaction  
 for 2 hr gave a mixture of (E) (III) and (Z)-2-MeC<sub>6</sub>H<sub>4</sub>CMe:CHPh (IV) and  
 2-MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>-CHPh(CH<sub>2</sub>)<sub>2</sub>S(O)Me. The reactions of I, its Z-isomer, II, III,  
 IV, and 2-MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CHPhCH<sub>2</sub>S(O)Me with MeS(O)C-H<sub>2</sub> are described. The  
 mechanism and apparent regiospecificity of methylation by MeS(O)C-H<sub>2</sub> are  
 explained.  
 IT **53423-30-6P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 53423-30-6 CAPLUS  
 CN Benzenepropanoic acid, 2-methyl- $\alpha$ -phenyl-, ethyl ester (9CI) (CA  
 INDEX NAME)



L13 ANSWER 26 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1974:107684 CAPLUS  
 DN 80:107684  
 TI Complex metal hydride reduction of carbon-carbon unsaturation. I. Sodium  
 borohydride reduction of  $\alpha$ -phenylcinnamates and related systems  
 AU Schauble, J. Herman; Walter, Gerald J.; Morin, J. Guy  
 CS USA  
 SO Journal of Organic Chemistry (1974), 39(6), 755-60  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DT Journal  
 LA English

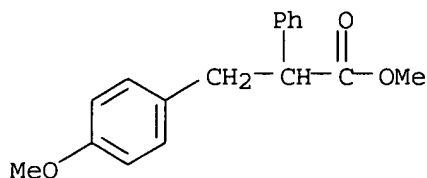
AB Competitive rates of NaBH<sub>4</sub> reduction for two sets of Me  $\alpha$ -phenyl-trans-cinnamates, para-substituted in the  $\alpha$  and  $\beta$  rings, resp., correlate linearly with Hammett substituent consts. The similarity in  $\rho_{\alpha}$  (1.74) and  $\rho_{\beta}$  (1.44) indicates that the transition state for hydride transfer occurs before significant change in geometry of the  $\alpha,\beta$ -unsatd. carbonyl system occurs. Competitive rate studies for Me  $\alpha$ -(para-substituted phenyl)acrylates and Me  $\alpha$ -phenyl-cis- and -trans-crotonates are corroborated by the data obtained for the cinnamates.

IT **5448-41-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 5448-41-9 CAPLUS

CN Benzenepropanoic acid, 4-methoxy- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 27 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1969:490560 CAPLUS

DN 71:90560

TI Kinetics of the decarboxylative dehydration of  $\beta$ -anisyl- $\beta$ -hydroxy- $\alpha$ -phenylpropionic acid

AU Noyce, Donald S.; McGoran, Ernest C.

CS Univ. of California, Berkeley, CA, USA

SO Journal of Organic Chemistry (1969), 34(9), 2558-61

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

AB The decarboxylative dehydrations of erythro- and threo- $\beta$ -anisyl- $\beta$ -hydroxy- $\alpha$ -phenylpropionic acids proceed at different rates in dilute aqueous H<sub>2</sub>SO<sub>4</sub>. Both stereoisomers give trans-4-methoxystilbene. The diastereoisomers are interconverted at a rate which is lower than decarboxylation in dilute H<sub>2</sub>SO<sub>4</sub>, but at a rate more rapid than decarboxylation in more acidic medium. These facts are interpreted in terms of generation of a dipolar ion which loses CO<sub>2</sub> more rapidly than it reacts with water.

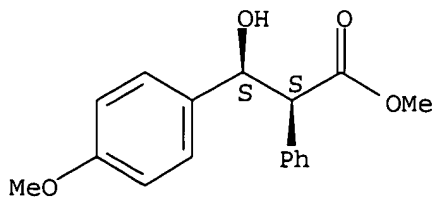
IT **20414-14-6P 20445-41-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 20414-14-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methoxy- $\alpha$ -phenyl-, methyl ester, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

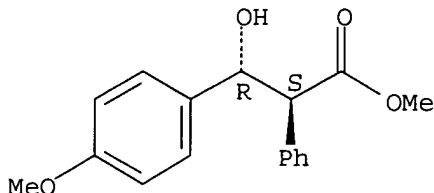


## CAS ONLINE PRINTOUT

RN 20445-41-4 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -hydroxy-4-methoxy- $\alpha$ -phenyl-, methyl ester, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 28 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1968:486787 CAPLUS

DN 69:86787

TI Heterocyclic compounds. Synthesis of  $\alpha$ -phenyl- $\beta$ -(4-methoxyphenyl)propionic esters; isomers of 1,2,5-trimethyl- and 1-allyl-2,5-dimethyl-4-piperidols

AU Sharifkanov, A. Sh.; Yusupov, S. A.; Starodubova, G.

CS USSR

SO Sb. Statei Aspir. Soiskatelei, Min. Vyssh. Sredn. Spets. Obrazov. Kaz. SSR, Khim. Khim. Tekhnol. (1966), 5, 164-7

From: Ref. Zh., Khim. 1967, Abstr. No. 22Zh330

DT Journal

LA Russian

GI For diagram(s), see printed CA Issue.

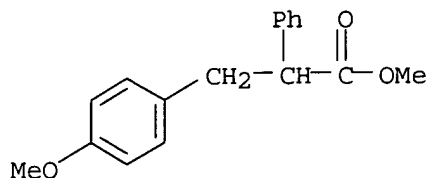
AB  $\alpha$ -Phenyl- $\beta$ -(4-methoxyphenyl)propionic esters of  $\alpha$ -isomers of 1,2,5-trimethyl- (I) and 1-allyl-2,5-dimethyl-4-piperidinols (II) were synthesized.  $\alpha$ -Phenyl- $\beta$ -(4-hydroxyphenyl)propionic acid (III) (12.1 g.) is added to a solution of 4 g. NaOH in 40 ml. of H<sub>2</sub>O while cooling, and after 1 hr., 13.8 g. Me<sub>2</sub>SO<sub>4</sub> is added. The solution is heated 3 hrs. in a bath at approx. 100° to give 80% Me  $\alpha$ -phenyl- $\beta$ -(4-methoxyphenyl)propionate (IV), b<sub>3</sub> 188-90°, m. 56-7°. III in ether with CH<sub>2</sub>N<sub>2</sub> gives 88.2% IV. A solution of 7.05 g. KOH in 126 ml. MeOH is added to a solution of 17 g. IV in 50 ml. MeOH and the mixture heated 1.5 hrs. at 60° to give 98.1% free acid (V), m. 121-2° (1:2 MeOH-H<sub>2</sub>O). A mixture of 16 g. V and 14.88 g. SOCl<sub>2</sub> is heated 1 hr. at 60° and 2 hrs. at 100-5° to give the acid chloride, m. 54-5°. A mixture of 2.14 g. of the  $\alpha$ -isomer of 1,2,5-trimethyl-4-piperidinol, 8.1 g. of the acid chloride, 0.1 g. Mg shavings, and 10 ml. dioxane is heated for 10 hrs. at 110-15° to give 54.8% VI.HCl, m. 61-2°. Under similar conditions, 2.5 g. of the  $\alpha$ -isomer of VII in 10 ml. dioxane, 0.1 g. Mg, and 8 g. of the acid chloride of V gave 87.3% VII.HCl, m. 49-51°. The acid chloride (10.4 g.) of VI is added to a solution of 3.4 g. II in 8 ml. pyridine and the mixture heated 12 hrs. at 125-30° to yield VII, 80.05%, VII, n<sub>D</sub><sup>20</sup> 1.5510.

IT 5448-41-9P

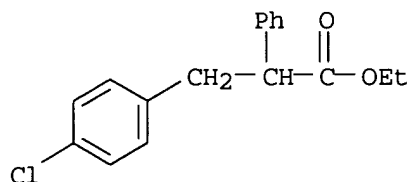
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 5448-41-9 CAPLUS

CN Benzenepropanoic acid, 4-methoxy- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



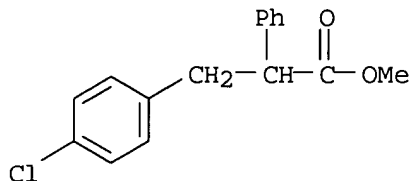
L13 ANSWER 29 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1965:462680 CAPLUS  
 DN 63:62680  
 OREF 63:11419b-d  
 TI Alkylations of phenylacetic,  $\alpha$ -alkylphenylacetic, and diphenyl-acetic esters by means of sodamide and sodium hydride  
 AU Kenyon, William G.; Kaiser, Edwin M.; Hauser, Charles R.  
 CS Duke Univ., Durham, NC  
 SO Journal of Organic Chemistry (1965), 30(9), 2937-42  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DT Journal  
 LA English  
 OS CASREACT 63:62680  
 AB Various alkylations of Et and tert-Bu phenyl-acetates with alkyl halides and further alkylations of the resulting  $\alpha$ -alkylphenylacetic esters were effected by means of sodamide in liquid ammonia. The method was successful even with p-chloro- and p-methoxyphenylacetic esters and with p-chlorobenzyl chloride. Typical alkylations were also effected by means of NaH in refluxing monoglyme. Sodamide was preferable for monoalkylations of Et or tert-Bu phenylacetates, but the 2 reagents were about equally effective for further alkylations of  $\alpha$ -alkylphenylacetic esters. NaH was better for dialkylation of Et phenylacetate with the same halide in a single operation. The present methods were superior to earlier methods. Also the present methods appear useful for the synthesis of certain mono- and dialkylarylacetic acids, which were obtained on hydrolysis of the alkylated esters. Et diphenylacetate was alkylated with certain halides by means of sodamide in liquid ammonia.  
 IT 3152-55-4, Propionic acid, 3-(p-chlorophenyl)-2-phenyl-, ethyl ester  
 (preparation of)  
 RN 3152-55-4 CAPLUS  
 CN Propionic acid, 3-(p-chlorophenyl)-2-phenyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



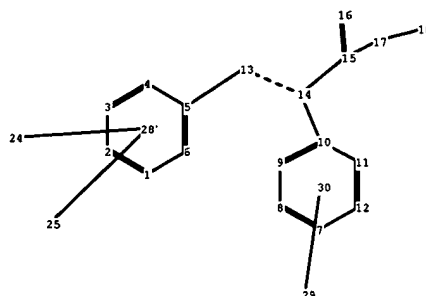
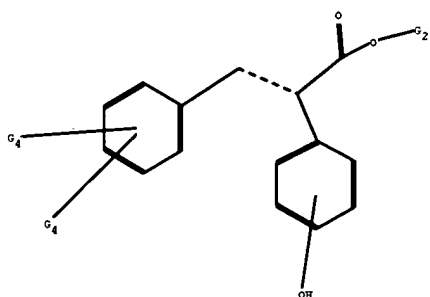
L13 ANSWER 30 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1963:408668 CAPLUS  
 DN 59:8668  
 OREF 59:1523d-e  
 TI Reactions of active methylene compounds in pyridine solution. V.  $\alpha$ -Hydroperoxy esters

## CAS ONLINE PRINTOUT

AU Avramoff, M.; Sprinzak, Y.  
 CS Weizmann Inst. Sci., Rehovoth, Israel  
 SO Journal of the American Chemical Society (1963), 85, 1655-7  
 CODEN: JACSAT; ISSN: 0002-7863  
 DT Journal  
 LA Unavailable  
 OS CASREACT 59:8668  
 AB cf. CA 55, 19858h. Base-catalyzed autoxidn. of esters of diarylacetic acids and 2,3-diarylpropionic acids affords  $\alpha$ -hydroperoxy esters  $\text{RCAr}(\text{OOH})\text{CO}_2\text{R}'$ , a novel type of hydroperoxides, along with  $\alpha$ -hydroxy esters and ketones. The formation of the latter two types of compds. is explained in terms of reduction and decomposition of the hydroperoxy esters.  
 IT 92907-23-8, Propionic acid, 3-(p-chlorophenyl)-2-phenyl-, methyl ester  
 (preparation of)  
 RN 92907-23-8 CAPLUS  
 CN Benzenepropanoic acid, 4-chloro- $\alpha$ -phenyl-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 31 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1959:44989 CAPLUS  
 DN 53:44989  
 OREF 53:8065f-i,8066a-b  
 TI Preparation of substituted  $\alpha,\beta$ -diphenylacrylic acids and related derivatives  
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 AB cf. C.A. 52, 9022a. Et  $\beta$ -(3,4-methylenedioxyphenyl)- $\alpha$ -phenylacrylate,  $\text{RR}_1\text{C}_6\text{H}_3\text{CH}:\text{CPhCO}_2\text{R}_2$  (I) ( $\text{RR}_1 = 3,4\text{-CH}_2\text{O}_2$ ,  $\text{R}_2 = \text{OEt}$ ) (II) (loc. cit.), was shown to be an excellent synergist for pyrethrum when tested against lice. Related compounds were prepared. The reported acrylic acids are trans compds. as indicated by m.p. data.  $p\text{-MeOC}_6\text{H}_4\text{CHO}$  and  $\text{PhCH}_2\text{CO}_2\text{H}$  condensed as previously described for the methylenedioxyphenyl compds. (loc. cit.), the crude acid (43%) stirred rapidly with 50% alc. at  $50^\circ$ , and the solution cooled gave  $p\text{-MeOC}_6\text{H}_4\text{CH}(\text{OH})\text{CHPhCO}_2\text{H}$  (III), m.  $136\text{-}8^\circ$  (decomposition). III (89 g.) and 50 g. anhydrous  $\text{NaOAc}$  stirred 4 hrs. in 200 ml.  $\text{Ac}_2\text{O}$  on a steam bath, the hot mixture poured onto 1 kg. cracked ice with stirring, kept overnight, and the water-washed precipitate recrystd. (95% alc.) yielded 75%  $p\text{-MeOC}_6\text{H}_4\text{CH}:\text{CHPh}$ , m.  $135\text{-}6^\circ$ . Similar decarboxylation of the corresponding  $3,4\text{-CH}_2\text{O}_2\text{C}_6\text{H}_3\text{CH}(\text{OH})\text{CHPhCO}_2\text{H}$  gave 97% I ( $\text{RR}_1 = 3,4\text{-CH}_2\text{O}_2$ ,  $\text{R}_2 = \text{OH}$ ) and not  $3,4\text{-CH}_2\text{O}_2\text{C}_6\text{H}_3\text{CH}:\text{CHPh}$  (IV). Crude  $\alpha$ -benzylpiperonyl alc. chrysanthemumate [cf. U.S. Dept. Agriculture ARS-33-42, Procedures C and E (1957)] distilled at  $145\text{-}80^\circ/0.2$  mm. in a short-path still gave a quant. yield of IV, m.  $93\text{-}4^\circ$  (95% alc.). MeO analogs of I were prepared as for II. I ( $\text{R} = \text{H}$ ,  $\text{R}_1 = o\text{-MeO}$ ,  $\text{R}_2 = \text{OH}$ ) (V), m.  $185\text{-}7^\circ$  (3:1 alc.- $\text{H}_2\text{O}$ ),



chain nodes :

13 14 15 16 17 18 24 25 29

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

5-13 10-14 13-14 14-15 15-16 15-17 17-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

13-14 15-16 15-17 17-18

exact bonds :

5-13 10-14 14-15

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,OH

G2:CH3,Et,n-Pr,i-Pr

G3:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,X

G4:MeO,EtO,n-PrO,i-PrO

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom  
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS  
18:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS